

A New Closed-Form Solution to Light Scattering by Spherical Nanoshells

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Abstract—Light or electromagnetic wave scattered by a single sphere or a coated sphere has been considered as a classic Mie theory. There have been some further extensions that were made further based on the Mie theory. Recently, a closed-form analytical model of the scattering cross section of a single nanoshell has been considered. The present paper is documented further, based on the work in 2006 by Alam and Massoud, to derive another different closed-form solution to the problem of light scattered by the nanoshells using polynomials of up to order 6. Validation is made by comparing the present closed-form solution to the exact Mie scattering solution and also to the other closed-form solution by Alam and Massoud. This study is found to be, however, more generalized and also more accurate for the coated spheres of either tiny/small or medium sizes than that of Alam and Massoud. Therefore, the derived formulas can be used for accurately characterizing both surface plasmon resonances of nanoparticles (of small sizes) or nanoantenna near-field properties (of medium sizes comparable with half wavelength).

Index Terms—Closed-form, light scattering, Mie theory, nanoshells.

I. INTRODUCTION

LIGHT scattering by spherical particles has been a classical subject that has attracted lots of interests over the past a few decades and was also formulated rigorously using the Mie theory [1]. Calculations of derivatives of Mie scattering coefficients were clearly shown in [2]. As the electrical parameter/size $k_0 a$ (where k_0 denotes the wavenumber of the free space and a stands for the radius of the sphere) of a scattering object becomes much smaller than 1, the Rayleigh scattering dominates [3], [4] and it is expressed approximately by the first-order expression in Mie scattering theory.

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Using the same method for matching boundary conditions, the results of electric and magnetic fields scattered by multilayered spherical structures can be easily extended [5]–[10].¹ Scattering of electromagnetic waves from two concentric spheres was first worked out by Aden and Kerker [5]. Scattering by multilayered spheres was well studied [6], [7] both in the near field and the far field. Scattering of an inhomogeneous sphere was also considered [8] where the sphere is discretized into a multilayered sphere of different permittivities along the radial direction. In addition, a sphere placed in a unbounded medium is also considered in [10], where how the incident plane wave is formulated and considered in the classical Mie scattering field theory was also addressed in detail. A number of applications was reported by Kerker [12].

Electromagnetic radiation problem associated with a multilayered sphere was also considered [13], [14]. The dyadic Green's functions used to define electric and magnetic fields in spherically multilayered media were derived [13], which helps to formulate the dipole or antenna radiation problem easily and straightforwardly. Applications of the electromagnetic radiation due to a loop antenna in the presence of a sphere was also considered [14], which could be applied to the medical radiation treatment to human head.

Light or electromagnetic scattering by composite spheres is another interest in the scientific and engineering communities [15]–[22]. Electromagnetic scattering by a plasma anisotropic sphere was analyzed [15]. The analysis was extended to Mie scattering by an uniaxial anisotropic sphere [16]. Furthermore, scattering by an inhomogeneous plasma anisotropic sphere of multilayers was also formulated and investigated [17]. It can be easily extended to light scattering by an inhomogeneous plasma anisotropic sphere where the exact solutions could be applied to obtain the field distributions in the multilayered spherical structures. Along the analysis line of [15]–[17], the standard eigenfunction expansion technique is utilized and the theory for the anisotropic media can still follow closely to theory used for the isotropic media. To characterize eigenvalues in the anisotropic media different from those in the isotropic media, potential formulation and parametric studies for scattering by rotationally symmetric anisotropic spheres were also carried out recently [18]. In addition, Sun discussed light scattering by coated sphere immersed in absorbing medium and compared finite-difference time-domain (FDTD) method with analytic solutions [19]. Scatterers consisting of concentric and nonconcentric multilayered spheres were also considered [20]. An

¹In case of [8], the full content appears in [9], and in case of [10], the full content appears in [11].

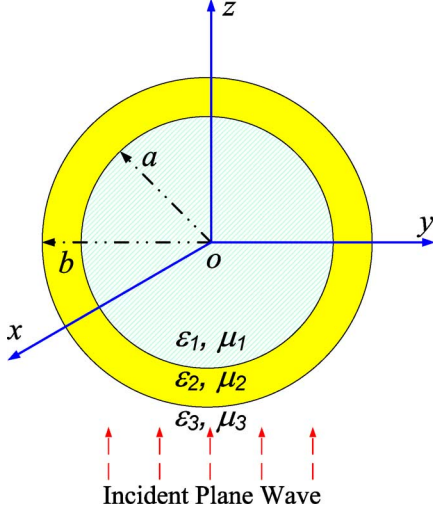


Fig. 1. Geometry of light scattering by a spherical nanoshell in hosting medium.

improved algorithm for electromagnetic scattering of plane wave and shaped beams by multilayered spheres was developed [21] and the geometrical-optics approximation of forward scattering by coated particles was then discussed [22].

With new developments of nanoscience and nanotechnology, it becomes desirable to investigate the microcosmic world of the scattering problems. Nanoscaled objects have thus attracted considerable attentions recently, primarily because they have shown some interesting optical properties and are found to be important for modern photonic applications [22]–[26]. Nanoscaled metallic particles exhibit interesting optical characteristics and behave differently from those of normal-scaled dimensions. Interactions of collective and individual particles of metals (such as copper, silver, and gold) were studied long time ago [27], [28]. Johnson and Christy plotted both the real and imaginary parts of relative permittivities of copper, silver, and gold nanoparticles as a function of photon energy in a large range according to different frequencies [29].

Recently, a closed-form analytical model of the scattering cross section of a single spherical nanoshell has been considered [30], while some fine experimental works were conducted in [31] and [32]. The results given in [30] seemed to agree with the exact solutions very well in accordance with the results in Figs. 2 and 3. Our recent careful investigations realize that the relative errors in their results are not so small, especially when the electric size of the nanoshell is not large. The present paper is therefore to derive another different closed-form solution for describing the lightwave scattered by the nanoshells using a polynomial of up to order 6. Validation will be made by comparing the present closed-form solution to the exact Mie scattering solution and also to the other closed-form solution by Alam and Massoud.

II. BASIC FORMULAS

The geometry of the problem defined in this paper is shown in Fig. 1, where we will follow closely with the definitions in [30]. So the outmost to innermost regions are denoted as

regions $i = 3, 2$, and 1 , whose permittivities and permeabilities are assumed to ϵ_i and $\mu_i = \mu_0$ (as nonmagnetic materials), respectively. The incident plane wave is propagating along $+z$ -direction. The inner radius of the coated sphere is a and outer radius is b ; in other words, the spherical geometrical thickness of the nanoshell is $c = b - a$. For convenience of the formulation, we take $x = k_0 a = \omega \sqrt{\epsilon_0 \mu_0} a = a\omega/c$ and $y = k_0 b = \omega \sqrt{\epsilon_0 \mu_0} b = b\omega/c$ to be the electrical parameters for the inner and outer radii of the spherical nanoshell (where c denotes the speed of light in free space).² It should be noted that here x and y are used to simplify the presentations and they have nothing to do with the Cartesian coordinates (x, y, z) . In addition, the refractive indexes of the spherical nanocore and the nanoshell are denoted by $m_1 = \sqrt{\epsilon_1/\epsilon_0}$ and $m_2 = \sqrt{\epsilon_2/\epsilon_0}$, respectively. The refractive index of the background hosting medium is $m_3 = \sqrt{\epsilon_3/\epsilon_0}$ and it is assumed herein that it is not necessarily unity, but it can be simplified as $m_3 = 1$ for free space. Correspondingly, the wavenumbers in the regions are denoted by $k_j = \omega \sqrt{\epsilon_j \mu_0}$, where $j = 1, 2$, and 3 , for the inner, the intermediate, and the outer regions of the problem geometry.

Electric field of an electromagnetic plane wave with an amplitude of E_0 in unbounded hosting medium can be written in terms of the spherical vector wave functions M (TE wave) and N (TM wave) as follows:

$$E_i = \sum_{n=1}^{\infty} i^n \frac{2n+1}{n(n+1)} \left(M_{o1n}^{(1)} - iN_{e1n}^{(1)} \right) \quad (1)$$

where an incident wave amplitude E_0 is assumed to be unity for simplification of the formulation. This assumption will not affect the further discussion and results. When it is scattered by the nanoshell, the electric wave outside of the nanoshell in the hosting medium is written in terms of the outgoing TE and TM waves in the following similar form:

$$E_{\text{scat},3} = \sum_{n=1}^{\infty} i^n \frac{2n+1}{n(n+1)} \left(a_n M_{o1n}^{(3)}(k_3 r) - i b_n N_{e1n}^{(3)}(k_3 r) \right) \quad (2a)$$

while the field inside the nanoshell is expressed by

$$E_{\text{scat},2} = \sum_{n=1}^{\infty} i^n \frac{2n+1}{n(n+1)} \left[\left(a'_n M_{o1n}^{(3)}(k_2 r) + c'_n M_{o1n}^{(1)}(k_2 r) \right) - i \left(b'_n N_{e1n}^{(3)} + d'_n N_{e1n}^{(1)} \right) \right] \quad (2b)$$

and the electric field inside the nanospherical core region is given due to the TE and TM standing waves by

$$E_{\text{scat},1} = \sum_{n=1}^{\infty} i^n \frac{2n+1}{n(n+1)} \left(c_n M_{o1n}^{(1)}(k_1 r) - i d_n N_{e1n}^{(1)}(k_1 r) \right). \quad (2c)$$

In the aforementioned field expressions, where the eigenvalue $m = 1$, the spherical vector wave functions $M_{emn}^{(i)}$ and $M_{omn}^{(i)}$ for even and odd TE modes, and $N_{emn}^{(i)}$ and $N_{omn}^{(i)}$ for even and

²The definition in [30] is not precisely correct unless the hosting or background medium is free space. Details of the proof will be given later.

odd TM modes are defined for $i = 1, 2, 3$, and 4 as

$$\begin{aligned} M_{emn}^{(i)}(kr) = & -z_n^{(i)}(\rho) \frac{mP_n^m(\cos\theta)}{\sin\theta} \sin m\phi \hat{\theta} \\ & - z_n^{(i)}(\rho) \frac{dP_n^m(\cos\theta)}{d\theta} \cos m\phi \hat{\phi} \end{aligned} \quad (3a)$$

$$\begin{aligned} M_{omn}^{(i)}(kr) = & z_n^{(i)}(\rho) \frac{mP_n^m(\cos\theta)}{\sin\theta} \cos m\phi \hat{\theta} \\ & - z_n^{(i)}(\rho) \frac{dP_n^m(\cos\theta)}{d\theta} \sin m\phi \hat{\phi} \end{aligned} \quad (3b)$$

$$\begin{aligned} N_{emn}^{(i)}(kr) = & \frac{n(n+1)z_n^{(i)}(\rho)}{\rho} P_n^m(\cos\theta) \cos m\phi \hat{r} \\ & + \frac{d}{\rho d\rho} [\rho z_n^{(i)}(\rho)] \left[\frac{dP_n^m(\cos\theta)}{d\theta} \cos m\phi \hat{\theta} \right. \\ & \left. - \frac{mP_n^m(\cos\theta)}{\sin\theta} \sin m\phi \hat{\phi} \right] \end{aligned} \quad (3c)$$

$$\begin{aligned} N_{omn}^{(i)}(kr) = & \frac{n(n+1)z_n^{(i)}(\rho)}{\rho} P_n^m(\cos\theta) \sin m\phi \hat{r} \\ & + \frac{d}{\rho d\rho} [\rho z_n^{(i)}(\rho)] \left[\frac{dP_n^m(\cos\theta)}{d\theta} \sin m\phi \hat{\theta} \right. \\ & \left. + \frac{mP_n^m(\cos\theta)}{\sin\theta} \cos m\phi \hat{\phi} \right]. \end{aligned} \quad (3d)$$

In the previous definitions, the superscripts (1), (2), (3), and (4) of $z_n^{(i)}(\rho)$ (where $\rho = kr$ denotes the argument of the spherical Bessel functions) refer to the first kind of spherical Bessel function, the second kind of spherical Bessel function, the first kind of spherical Hankel function, and the second kind of spherical Hankel function, respectively.

Apparently, there exist eight sets of unknown parameters, $(a_n, b_n, c_n, \text{ and } d_n)$ and also $(a'_n, b'_n, c'_n, \text{ and } d'_n)$, to be determined. From continuity relations of electric field and magnetic field tangential components, we will have four boundary conditions on the inner spherical interface and the other four boundary conditions on the outer spherical interface. So, all the unknown coefficients can be determined uniquely. The solution procedure is rather standard, although lengthy. So, we will not provide the details of all the solutions, instead we will provide the obtained scattering coefficients in the hosting medium only, a_n and b_n . They are given by

$$a_n = \frac{a_n^{\text{num}}}{a_n^{\text{den}}} \quad \text{and} \quad b_n = \frac{b_n^{\text{num}}}{a_n^{\text{den}}} \quad (4)$$

where the numerators $N_n^{a,b}$ and denominators $D_n^{a,b}$ of the two scattering coefficients are explicitly given as follows:

$$\begin{aligned} a_n^{\text{num}} = & m_3 \psi_n(m_3 y) [\psi'_n(m_2 y) - A_n \chi'_n(m_2 y)] \\ & - m_2 \psi'_n(m_3 y) [\psi_n(m_2 y) - A_n \chi_n(m_2 y)] \end{aligned} \quad (5a)$$

$$\begin{aligned} a_n^{\text{den}} = & m_3 \xi_n(m_3 y) [\psi'_n(m_2 y) - A_n \chi'_n(m_2 y)] \\ & - m_2 \xi'_n(m_3 y) [\psi_n(m_2 y) - A_n \chi_n(m_2 y)] \end{aligned} \quad (5b)$$

$$\begin{aligned} b_n^{\text{num}} = & m_2 \psi_n(m_3 y) [\psi'_n(m_2 y) - B_n \chi'_n(m_2 y)] \\ & - m_3 \psi'_n(m_3 y) [\psi_n(m_2 y) - B_n \chi_n(m_2 y)] \end{aligned} \quad (5c)$$

$$\begin{aligned} a_n^{\text{den}} = & m_2 \xi_n(m_3 y) [\psi'_n(m_2 y) - B_n \chi'_n(m_2 y)] \\ & - m_3 \xi'_n(m_3 y) [\psi_n(m_2 y) - B_n \chi_n(m_2 y)] \end{aligned} \quad (5d)$$

with the intermediate parameters A_n and B_n defined³ as

$$A_n = \frac{m_2 \psi_n(m_2 x) \psi'_n(m_1 x) - m_1 \psi'_n(m_2 x) \psi_n(m_1 x)}{m_2 \chi_n(m_2 x) \psi'_n(m_1 x) - m_1 \chi'_n(m_2 x) \psi_n(m_1 x)} \quad (6a)$$

$$B_n = \frac{m_2 \psi_n(m_1 x) \psi'_n(m_2 x) - m_1 \psi'_n(m_1 x) \psi_n(m_2 x)}{m_2 \chi'_n(m_2 x) \psi_n(m_1 x) - m_1 \chi_n(m_2 x) \psi'_n(m_1 x)} \quad (6b)$$

and the Riccati–Bessel functions were defined⁴ as

$$\psi_n(\rho) = \rho j_n(\rho) \quad (7a)$$

$$\chi_n(\rho) = \rho y_n(\rho) \quad (7b)$$

$$\xi_n(\rho) = \rho h_n^{(1)}(\rho) = \rho [j_n(\rho) + i y_n(\rho)] \quad (7c)$$

with the prime to denote their first-order derivative of the Riccati–Bessel functions. For the nonmagnetic medium, we have the free-space permeability for all the regions, i.e., $\mu_1 = \mu_2 = \mu_3 = \mu_0$. Again, ϵ_1 and ϵ_2 denote the permittivities of the spherical nanocore and the nanoshell, while ϵ_3 stands for the permittivity in the outer region of the structure. The formulas given in (5a)–(5d) are slightly different from those forms in [30], because we herein enclose m_3 in the formulation without loss of any generality while the formulas [30, eqs. (1) and (2)] are only applicable to the case where the outer region is free space; but in the later applications in [30], the authors assumed $\epsilon_3 = 1.78\epsilon_0$.

III. NEW CLOSED-FORM SOLUTION TO INTERMEDIATE COEFFICIENTS A_n AND B_n

As the scattering coefficients a_n and b_n are of our specific interests here, although they look very complicated and involved with the spherical Bessel functions of various kinds. To do so, we also follow the similar procedure of approximating the scattering coefficients a_n and b_n by taking the series expansions of the following first and second kinds of spherical Bessel functions as follows:

$$\begin{aligned} j_n(z) = & \frac{z^n}{(2n+1)!!} \\ & \times \left[1 - \frac{z^2/2}{1!(2n+3)} + \frac{(z^2/2)^2}{2!(2n+3)(2n+5)} + \cdots \right] \end{aligned} \quad (8a)$$

$$\begin{aligned} y_n(z) = & \frac{(2n-1)!!}{z^{n+1}} \\ & \times \left[1 - \frac{z^2/2}{1!(1-2n)} + \frac{(z^2/2)^2}{2!(1-2n)(3-2n)} + \cdots \right] \end{aligned} \quad (8b)$$

where, and subsequently, $n!!$ denotes the factorial by a step of 2 (for instance, $7!! = 7 \cdot 5 \cdot 3 \cdot 1$ while $8!! = 8 \cdot 6 \cdot 4 \cdot 2$). The

³Subscripts of some $\psi_n(\rho)$ and its derivative were missing in [30, eqs. (12) and (13)].

⁴ $\chi_n(\rho)$ was not generally defined in [30].

numerical tests show that when $x = 0.6$ and $n = \{1, 2, 3\}$, we will have the following exact values of $j_n(z) = \{0.192892, 0.023389, 0.00201634\}$. If we use the approximation in [30], the following values are obtained: $j_n(z) = \{0.149956, 0.0196055, 0.00175972\}$; but if we use the approximations in (8a) and (8b) of this paper where only the explicit first three terms are included, we will obtain fairly accurate results of $j_n(z) = \{0.192893, 0.023389, 0.00201634\}$. Similarly, for the same given conditions ($x = 0.6$ and $n = \{1, 2, 3\}$), we have the exact values of $y_n(z) = \{3.23367, 14.7928, 120.04\}$, the approximate values of $y_n(z) = \{3.95662, 24.7842, 155.333\}$ by [30], and the approximate values of $y_n(z) = \{3.23278, 14.7972, 120.032\}$ by this paper.

A. Approximate Expression of Coefficient A_n

With the confidence built, we are now moving toward deriving the closed-form solution for the coefficient A_n as follows:

$$A_n \approx \frac{A_n^{\text{num}}}{A_n^{\text{den}}} \quad (9)$$

where we have the closed-form solutions to the numerator A_n^{num} and denominator A_n^{den} as follows:

$$\begin{aligned} A_n^{\text{num}} = & -(2n-5)(2n-3)(2n-1)\pi x^{2n+1} m_2^{2n+1} (m_2^2 \\ & - m_1^2) \{x^4 (4n^3 + 24n^2 + 41n - 2x^2 m_2^2 + 21) m_1^4 \\ & - 2x^2 [x^4 m_2^4 - (4n^3 + 28n^2 + 67n + 63) x^2 m_2^2 \\ & + 2(8n^4 + 68n^3 + 202n^2 + 247n + 105)] m_1^2 \\ & + (4n^3 + 24n^2 + 41n + 21) [x^4 m_2^4 - 4(2n+5) \\ & \times x^2 m_2^2 + 8(4n^2 + 16n + 15)]\} \end{aligned} \quad (10a)$$

$$\begin{aligned} A_n^{\text{den}} = & 4^n (4n^2 + 8n + 3) \Gamma^2 \left(n + \frac{1}{2} \right) \{ (4n^2 + 24n \\ & + 35) x^4 [4n^3 - 19n + (1-2n)x^2 m_1^2 - 15] m_2^6 \\ & + (4n^2 + 4n - 35) x^2 [2(2n+1)x^4 m_1^4 - (4n^3 \\ & + 32n^2 + 43n - 30) x^2 m_1^2 + 4(8n^4 + 28n^3 + 2n^2 \\ & - 63n - 45)] m_2^4 + (4n^2 - 16n + 15) [-(2n+3) \\ & \times x^6 m_1^6 + (-4n^3 + 79n + 105) x^4 m_1^4 - 12(8n^3 \\ & + 52n^2 + 94n + 35) x^2 m_1^2 + 8(16n^5 + 128n^4 \\ & + 336n^3 + 292n^2 - 37n - 105)] m_2^2 + n(16n^4 \\ & - 16n^3 - 160n^2 + 292n - 105) m_1^2 [x^4 m_1^4 - 4(2n \\ & + 5)x^2 m_1^2 + 8(4n^2 + 16n + 15)]\} \end{aligned} \quad (10b)$$

It is noted that a factor of

$$F_n^A = \frac{m_1^n (32n^5 + 48n^4 - 400n^3 - 216n^2 + 1250n - 525)^{-1}}{128 \times 2^{2n} \times m_2^{n+1} \times \Gamma^2(n + (5/2))} \quad (11)$$

has been involved in both the numerator and the denominator of coefficient A_n in (6a) and has been canceled in (9).

It is seen that the solution derived here is general enough for all the different values of n and x values, more complete in form than that given in [30]. Also, it is seen that the closed-form solution is very simple, given in terms of only some simple additions of algebraic functions. Also, it is to be shown later that they are quite accurate; and it is valid for complex argument x as well. For those who use Fortran or C language to write their own codes for computations, this has made the code implementation extremely easier and faster.

Specifically, we need to generate the solution for the first few orders. First, we have the case of $n = 1$, and easily we have the following simplified solution:

$$\begin{aligned} A_1^{\text{num}} = & 27\pi x^3 m_2^3 (m_1^2 - m_2^2) [2800 - 280(m_1^2 + m_2^2) x^2 \\ & + (10m_1^4 + 36m_2^2 m_1^2 + 10m_2^4) x^4] \end{aligned} \quad (12a)$$

$$\begin{aligned} A_1^{\text{den}} = & \frac{15\pi}{4} [30240(m_1^2 + 2m_2^2) - 3024(m_1^2 - m_2^2)(m_1^2 \\ & + 10m_2^2) x^2 + 4(27m_1^6 + 540m_2^2 m_1^4 + 1323m_2^4 m_1^2 \\ & - 1890m_2^6) x^4 + 4(-15m_2^2 m_1^6 - 162m_2^4 m_1^4 \\ & - 63m_2^6 m_1^2) x^6] \end{aligned} \quad (12b)$$

and when $n = 2$

$$\begin{aligned} A_2^{\text{num}} = & -33\pi x^5 m_2^5 (m_1^2 - m_2^2) [10584 - 756(m_1^2 + m_2^2) \\ & \times x^2 + (21m_1^4 + 62m_2^2 m_1^2 + 21m_2^4) x^4] \end{aligned} \quad (13a)$$

$$\begin{aligned} A_2^{\text{den}} = & \frac{315\pi}{16} [-266112(2m_1^2 + 3m_2^2) + 6336(m_1^2 - m_2^2) \\ & (6m_1^2 + 21m_2^2) x^2 + 16(-66m_1^6 - 231m_2^2 m_1^4 \\ & + 2376m_2^4 m_1^2 - 2079m_2^6) x^4 + 16(7m_2^2 m_1^6 \\ & - 110m_2^4 m_1^4 - 297m_2^6 m_1^2) x^6] \end{aligned} \quad (13b)$$

B. Approximate Expression of Coefficient B_n

Similarly, the closed-form solution for the coefficient B_n is given by

$$B_n \approx \frac{B_n^{\text{num}}}{B_n^{\text{den}}} \quad (14)$$

where we have the following closed-form solutions to the numerator B_n^{num} and denominator B_n^{den} :

$$\begin{aligned} B_n^{\text{num}} = & (128n^7 + 448n^6 - 1120n^5 - 3920n^4 + 2072n^3 \\ & + 7252n^2 - 450n - 1575) \pi x^{2n+3} m_2^{2n+1} (m_1^2 \\ & - m_2^2) \{ (2n+3)x^4 m_1^4 + 2x^2 [(2n+5)x^2 m_2^2 \\ & - 4(4n^2 + 20n + 21)] m_1^2 + (2n+3) [x^4 m_2^4 \\ & - 8(2n+7)x^2 m_2^2 + 16(4n^2 + 24n + 35)] \} \end{aligned} \quad (15a)$$

$$\begin{aligned} B_n^{\text{den}} = & 4^n (2n+1)^2 (2n+3)^2 (4n^2 + 24n + 35) \\ & \times \Gamma^2 \left(n + \frac{1}{2} \right) \{ -(8n^3 - 36n^2 + 46n - 15) \\ & \times x^6 m_1^6 + (8n^3 - 4n^2 - 82n + 105) x^4 (8n^2 \end{aligned}$$

$$\begin{aligned}
& + 16n + x^2 m_2^2 - 10) m_1^4 - (8n^3 + 28n^2 - 50n \\
& - 175) x^2 [-x^4 m_2^4 + 4(4n^2 - 4n - 3) x^2 m_2^2 \\
& + 8(8n^3 - 4n^2 - 18n + 9)] m_1^2 + (8n^3 + 60n^2 \\
& + 142n + 105) [-x^6 m_2^6 + 2(4n^2 - 16n + 15) \\
& \times x^4 m_2^4 + 8(8n^3 - 36n^2 + 46n - 15) x^2 m_2^2 \\
& + 16(16n^4 - 64n^3 + 56n^2 + 16n - 15)] \}. \quad (15b)
\end{aligned}$$

Similarly, it is also noted that a factor of

$$F_n^B = \frac{2^{-2(n+6)} m_1^{n+1} m_2^{-n}}{(2n-5)(2n-3)(2n-1)(2n+1)(2n+3)\Gamma^2(n+(9/2))} \quad (16)$$

has been involved in both the numerator and the denominator of coefficient B_n in (6b) and has been canceled in (14).

To make it applicable and specific in solution, we consider the solution to the coefficient B_1 next. Again, we split its expression into the numerator and denominator and they are respectively given as follows:

$$B_1^{\text{num}} = -x^5 m_2^3 (m_1^2 - m_2^2) \{ [5x^2 m_1^4 + 2(7x^2 m_2^2 - 180) \times m_1^2 + 5m_2^2 (x^2 m_2^2 - 72)] x^2 + 5040 \} \quad (17a)$$

$$\begin{aligned}
B_1^{\text{den}} = & 15 [x^6 m_1^6 - 9x^4 (x^2 m_2^2 + 14) m_1^4 + 63x^2 (x^4 m_2^4 \\
& + 12x^2 m_2^2 + 40) m_1^2 + 105 (x^6 m_2^6 - 6x^4 m_2^4 \\
& - 24x^2 m_2^2 - 144)] \}. \quad (17b)
\end{aligned}$$

The previous fractional form suggests that the solution to the coefficient B_1 is not as simple as the expression of the linear function of x^5 given in [30]. To gain more insight into the accuracy of the expressions, we will discuss on the details of comparisons among the three sets of data, the exact solution from Mie theory, the closed-form solution in [30], and the new closed-form solution in this paper.

C. Validations and Accuracy

To gain insight into the accuracy of the present closed-form solution to the coefficients A_n and B_n , we have considered relative errors of the numerical results obtained using the present closed-form solution as compared with the exact results obtained directly from the Mie scattering theory. In addition, we have also considered the relative errors of the previously obtained closed-form solution results in [30]. To gain the consistent results, we also assume the same parameters as used in [30], where $\epsilon_1 = (5.44/1.78)\epsilon_0$, $\epsilon_3 = \epsilon_0$, and $\epsilon_2 = (\epsilon_1 + \epsilon_3)/2$. A comparison has been shown in Fig. 2(a) for the coefficient A_1 , in Fig. 2(b) for the coefficient A_2 , and in Fig. 2(c) for the coefficient B_1 . It is clearly shown that the present results of closed-form solution to these coefficients are far more accurate than those in [30] where the relative error of A_1 is always larger than 25% and can reach 30%; the relative error of A_2 increase up to 25% at a speed faster than cubic power; and the relative error of B_1 also increases from 17% to 35%.

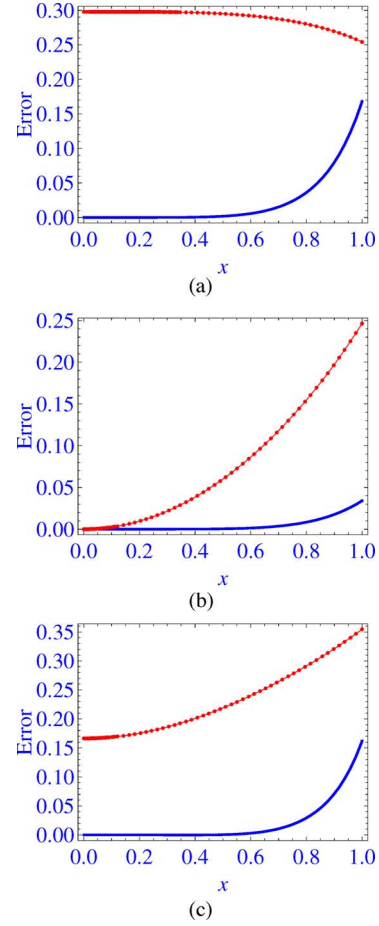


Fig. 2. Relative errors of coefficients A_1 , A_2 , and B_1 obtained in this paper and also in [30], all compared with the exact solution obtained using the Mie scattering theory. The bullet-dotted curve “—•—” denotes the results in [30] while the solid curve “—” stands for the result in this paper. (a) Coefficient A_1 . (b) Coefficient A_2 . (c) Coefficient B_1 .

IV. NEW CLOSED-FORM SOLUTIONS TO SCATTERING COEFFICIENTS a_n AND b_n

Now, we turn to the approximations finally to the scattering coefficients a_n and b_n . Substituting (8a) and (8b) into (7a) and (7b) and further into (7c), we could approximate (5a) and (5b) as follows.

A. Approximate Expression of Coefficient a_n

1) *Generalized Case for Any n and Arbitrary Material Properties*: Without loss of any generality, we would keep all the intermediates inside. From the Taylor series expansions and keeping the terms up to the order 6, we have

$$a_n = y^{2n+1} \frac{\alpha_{n,n}}{\alpha_{n,d}} = y^{2n+1} \frac{\sum_{\ell=0}^6 \alpha_{n,n}^{(\ell)} y^\ell}{\sum_{\ell=0}^6 \alpha_{n,d}^{(\ell)} y^\ell} \quad (18)$$

where the coefficients for the numerator are

$$\alpha_{n,n}^{(0)} = -A_n m_2^{-n-1} m_3^n \frac{(n+1)m_2^2 + nm_3^2}{2n+1} \quad (19a)$$

$$\alpha_{n,n}^{(1)} = 0 \quad (19b)$$

$$\alpha_{n,n}^{(2)} = A_n m_2^{-n-1} m_3^n (m_3^2 - m_2^2) \times \frac{(2n^2 + 5n + 3) m_2^2 + n(2n - 1) m_3^2}{2(8n^3 + 12n^2 - 2n - 3)} \quad (19c)$$

$$\alpha_{n,n}^{(3)} = -\frac{4^{-n}(n+1)\pi m_2^n m_3^n (m_2^2 - m_3^2)}{(2n+1)^2 \Gamma^2(n+1/2)} y^{2(n-1)} \quad (19d)$$

$$\alpha_{n,n}^{(4)} = A_n m_2^{-n-1} m_3^n (m_3^2 - m_2^2) [(n+1)(2n+3)(2n+5)m_2^4 - 3[4n(n+1) - 15]m_3^2 m_2^2 - n[4n(n-2) + 3]m_3^4] / [8(4n^2 - 9)(4n^2 - 1)(2n+5)] \quad (19e)$$

$$\alpha_{n,n}^{(5)} = \frac{2^{-2n-1}(n+1)\pi m_2^n m_3^n (m_2^4 - m_3^4)}{(2n+1)^2(2n+3)\Gamma^2(n+1/2)} y^{2(n-1)} \quad (19f)$$

$$\alpha_{n,n}^{(6)} = A_n m_2^{1-n} m_3^{n+2} [(2n-1)(2n+5)(2n+7)m_2^4 - 2(2n-5)(2n+1)(2n+7)m_3^2 m_2^2 + (2n-5)(2n-3)(2n+3)m_3^4] / [8(4n^2 - 25)(4n^2 - 9) \times (4n^2 - 1)(2n+7)] \quad (19g)$$

while the coefficients for the denominator are

$$\alpha_{n,d}^{(0)} = -\frac{i4^n n}{\pi} \Gamma^2\left(n + \frac{1}{2}\right) A_n m_2^{-n-1} m_3^{-n-1} (m_2^2 - m_3^2) \quad (20a)$$

$$\alpha_{n,d}^{(1)} = 0 \quad (20b)$$

$$\alpha_{n,d}^{(2)} = -\frac{i2^{2n-3}n}{\pi} (2n-1)\Gamma^2\left(n - \frac{1}{2}\right) A_n \times m_2^{-n-1} m_3^{-n-1} (m_2^4 - m_3^4) \quad (20c)$$

$$\alpha_{n,d}^{(3)} = \frac{y^{2(n-1)} m_2^{-n-1} m_3^{-n-1}}{2n+1} \{-i[nm_2^2 + (n+1)m_3^2] \times m_2^{2n+1} - A_n m_3^{2n+1} [(n+1)m_2^2 + nm_3^2]\} \quad (20d)$$

$$\alpha_{n,d}^{(4)} = -\frac{i2^{2n-3}}{(1-2n)^2(2n-3)\pi} \Gamma^2\left(n + \frac{1}{2}\right) A_n m_2^{-n-1} \times m_3^{-n-1} (m_2^2 - m_3^2) \{n(2n-1)m_2^4 + 2[n(2n-3) + 4]m_3^2 m_2^2 + n(2n-1)m_3^4\} \quad (20e)$$

$$\alpha_{n,d}^{(5)} = \frac{y^{2(n-1)} m_2^{-n-1} m_3^{-n-1}}{2(4n^2 - 1)(2n+3)} (m_2^2 - m_3^2) [i(n+1)(2n+3)m_3^2 m_2^{2n+1} + in(2n-1)m_2^{2n+3} - (n+1) \times (2n+3)A_n m_3^{2n+1} m_2^2 - n(2n-1)A_n m_3^{2n+3}] \quad (20f)$$

$$\alpha_{n,d}^{(6)} = -\frac{i4^{n-4}}{\pi} [4(n-4)n + 15]\Gamma^2\left(n - \frac{5}{2}\right) A_n m_2^{1-n} \times (m_2^4 - m_3^4) m_3^{1-n} - \frac{4^{-n-1}(n+1)\pi y^{4(n-1)} m_2^n}{\Gamma^2(n+3/2)} \times (m_2^2 - m_3^2) m_3^n. \quad (20g)$$

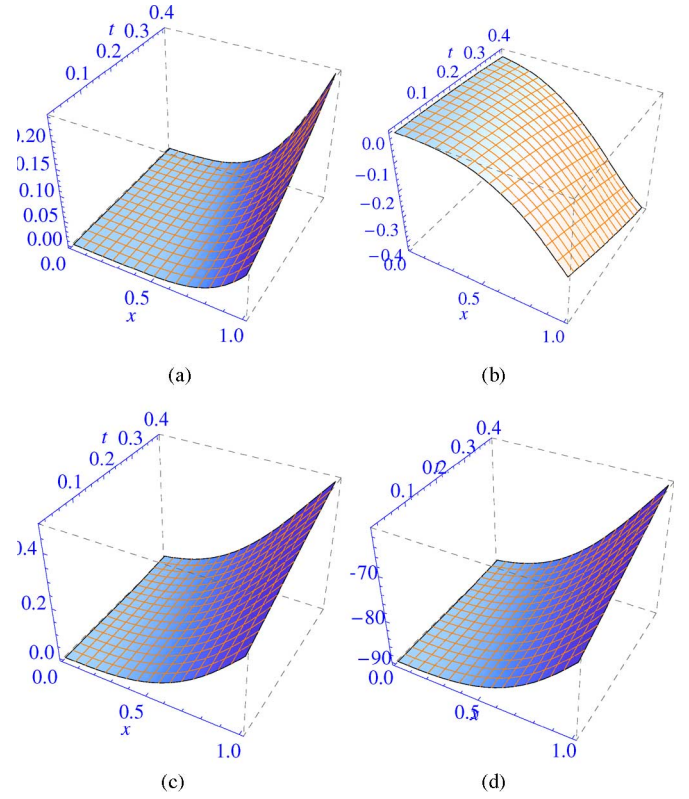


Fig. 3. Exact coefficient a_1 versus the spherical core radius $x \in (0.01, 1.0)$ and the spherical nanoshell thickness $t \in (0.01, 0.4)$. The other electrical parameters are $\epsilon_1 = (5.44/1.78)\epsilon_0$, $\epsilon_3 = \epsilon_0$, and $\epsilon_2 = (\epsilon_1 + \epsilon_3)/2$, while $\mu_1 = \mu_2 = \mu_3 = \mu_0$. (a) Real part of a_1 . (b) Imaginary part of a_1 . (c) Magnitude of a_1 . (d) Phase (in degrees) of a_1 .

These coefficients look complicated, because we considered the general cases of the materials and also the expansion polynomial series up to power 6. They could be significantly simplified, as will be demonstrated later. It should be noted that the expressions of numerator and denominator in (18) do not simply follow the power series exactly because the order number n involves also in the power series. For instance, $y^{2(n-1)}$ and $y^{4(n-1)}$ are contained in the intermediate series coefficients, but they will disappear when the first order $n = 1$ is considered. When the second or higher orders are considered, then we have to see if they should be excluded because we basically keep the series expansion up to the order 6.

To see the general variation of the coefficient a_n , we look into the first and dominant coefficient a_1 and plotted their real [see Fig. 3(a)] and imaginary [see Fig. 3(b)] parts in Fig. 3, of which the real part is directly used to calculate the extinction cross sections. It is shown that they change monotonically within the range of the electrical spherical core radius $x \in (0.01, 1.0)$ and the electrical spherical nanoshell radius $y = x + t \in (0.02, 1.4)$ where the spherical nanoshell thickness $t \in (0.01, 0.4)$. As the scattering cross section involves the magnitude, therefore we also consider the magnitude [see Fig. 3(c)] and phase [in degrees in Fig. 3(d)] variations of the coefficient a_1 . It is clearly seen that within the ranges of the physical parameters, these variations are also monotonic. These provide certain sense for the accuracy versus the expansion order of the coefficients, and thus confirm the feasibility of this study.

2) *Special Case I* ($n = 1$): To simplify the previous expression of a_n , we let $n = 1$ but still leave m_3 to be general. Therefore, the following significantly simplified terms are obtained:

$$a_1 = y^3 \frac{\alpha_{1,n}}{\alpha_{1,d}} \quad (21)$$

where

$$\begin{aligned} \alpha_{1,n} = & -\frac{A_1 m_3}{3} (2m_2^2 + m_3^2) + \frac{A_1 m_3}{30} (-10m_2^4 \\ & + 9m_3^2 m_2^2 + m_3^4) y^2 - \frac{2m_2^3 m_3}{9} (m_2^2 - m_3^2) y^3 \\ & - \frac{A_1 m_3}{840} (-70m_2^6 + 49m_3^2 m_2^4 + 20m_3^4 m_2^2 \\ & + m_3^6) y^4 - \frac{m_3}{45} (m_2^3 m_3^4 - m_2^7) y^5 \\ & + \frac{A_1 m_2^2 m_3^3}{7560} (21m_2^4 + 54m_3^2 m_2^2 + 5m_3^4) y^6 \end{aligned} \quad (22a)$$

$$\begin{aligned} \alpha_{1,d} = & \frac{iA_1}{m_3^2} (m_3^2 - m_2^2) + \frac{iA_1}{2m_3^2} (m_3^4 - m_2^4) y^2 \\ & - \frac{1}{3} \left(\frac{im_2^5}{m_3^2} + 2im_2^3 + 2A_1 m_3 m_2^2 + A_1 m_3^3 \right) y^3 \\ & + \frac{iA_1 (m_2^6 + 5m_3^2 m_2^4 - 5m_3^4 m_2^2 - m_3^6)}{8m_3^2} y^4 \\ & + \frac{i(m_2^2 - m_3^2)}{30m_3^2} (m_2^5 + 10m_3^2 m_2^3 + 10iA_1 m_3^3 m_2^2 \\ & + iA_1 m_3^5) y^5 + \frac{1}{36} m_2^2 [-8m_3 m_2^3 + 8m_3^3 m_2 \\ & - 3iA_1 (m_2^4 - m_3^4)] y^6. \end{aligned} \quad (22b)$$

In (21) together with (22a) and (22b), the intermediate parameter A_1 was defined in (9) (where $n = 1$) together with their numerator and denominator defined in (12a) and (12b), respectively. Please note that the previous specific coefficients in (21) given in (22a) and (22b) can be directly simplified from the expression in (18) except for the cancellation of a factor m_2^2 in both denominators of $\alpha_{1,n}$ and $\alpha_{1,d}$. The coefficient a_1 shown in (21) together with its intermediate coefficients in (22a) and (22b) can be simplified by letting $m_3 = 1$, the same as what was done in [30]. Doing so, we could further simplify the expressions.

After the approximate coefficient a_1 is obtained, we may wish to validate it and confirm its accuracy range versus the *electrical* inner radius $x \in (0.01, 1.0)$ and *electrical* outer radius y of the spherical nanoshell. For ease of understanding and calculation, we consider the nanoshell thickness $t \in (0.01, 0.4)$ to represent the outer radius $y = x + t \in (0.02, 1.4)$, as shown in Fig. 4. When we consider the relative error limit of 0.68 for the real part of coefficient $\text{Re}[a_1]$, it is seen in Fig. 4(a) that the maximum relative error of this study is below 0.68, while it is much smaller for scientific and engineering applications when the nanocore radius is not electrically large or when the nanoshell is not electrically thick. At the meantime, we limit the same relative error of 0.68 for the results in [30] and it is seen that the inaccurate area (as cut on the top of the 3-D

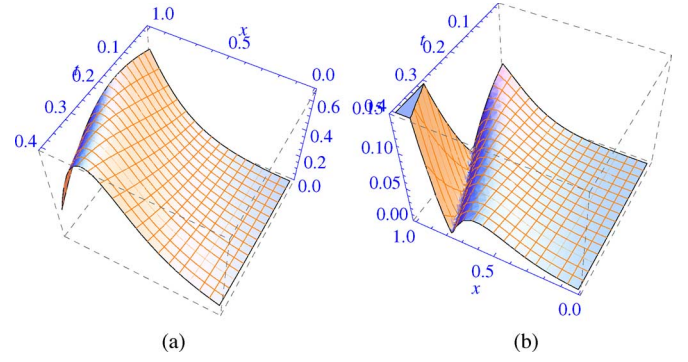


Fig. 4. Relative errors (with respect to the exact solution) of approximate coefficient a_1 formulas derived here in this paper versus the spherical core radius $x \in (0.01, 1.0)$ and the spherical nanoshell thickness $t \in (0.01, 0.4)$. The other electrical parameters used here are the same as those in Figs. 2 and 3, and they will be used for the future numerical results, and thus omitted later. (a) Error of $\text{Re}[a_1]$ here. (b) Error of $|a_1|$ here.

figure) becomes very large. There is only a small region where the relative error of $\text{Re}[a_1]$ in [30] is smaller than 0.68. As the scattering cross section is proportional to the magnitude square of the coefficient, $|a_1|^2$, therefore, we also look into the relative errors of $|a_1|$ in this paper and also the work in [30], but limit both of them to the allowable errors of 0.15 for engineering applications. It is found from Fig. 4(b) that the approximate results produced in this paper are fairly accurate. For the results produced in this paper, there is only a very small inaccurate area with relative error slightly larger than 0.15, as shown in Fig. 4(b).

3) *Special Case II* ($n = 2$): Similarly, we could also simplify the previous general expression of a_n by letting $n = 2$ to obtain the coefficient a_2 . As a result, the following simplified formula is obtained:

$$a_2 = y^5 \frac{\alpha_{2,n}}{\alpha_{2,d}} \quad (23)$$

where

$$\begin{aligned} \alpha_{2,n} = & -\frac{1}{5} A_2 m_3^2 (3m_2^2 + 2m_3^2) + \frac{1}{70} A_2 m_3^2 (-7m_2^4 \\ & + 5m_3^2 m_2^2 + 2m_3^4) y^2 - \frac{A_2 m_3^2}{2520} (63m_2^6 - 72m_3^2 m_2^4 \\ & + 7m_3^4 m_2^2 + 2m_3^6) y^4 - \frac{1}{75} m_2^5 m_3^2 (m_2^2 - m_3^2) y^5 \\ & - \frac{A_2 m_2^2 m_3^4}{83160} (297m_2^4 + 110m_3^2 m_2^2 - 7m_3^4) y^6 \end{aligned} \quad (24a)$$

$$\begin{aligned} \alpha_{2,d} = & \frac{18iA_2}{m_3^3} (m_3^2 - m_2^2) + \frac{3iA_2}{m_3^3} (m_3^4 - m_2^4) y^2 + \frac{3iA_2}{4m_3^3} \\ & \times (m_3^2 - m_2^2) (m_2^2 + m_3^2)^2 y^4 - \frac{1}{5m_3^3} (2im_2^7 \\ & + 3im_3^2 m_2^5 + 3A_2 m_3^5 m_2^2 + 2A_2 m_3^7) y^5 + \frac{iA_2 m_2^2}{4m_3} \\ & \times (m_2^4 - m_3^4) y^6. \end{aligned} \quad (24b)$$

In (23) together with (24a) and (24b), the intermediate parameter A_2 was defined in (9) (where $n = 2$) together with

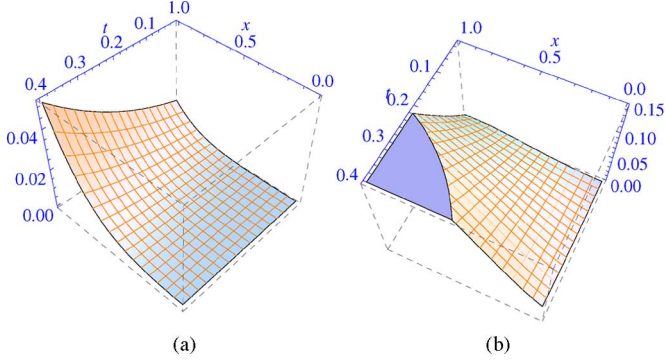


Fig. 5. Variation of $|a_2|$ and the relative error (with respect to the exact solution) of the formulas derived in this paper versus the spherical core radius $x \in (0.01, 1.0)$ and the spherical nanoshell thickness $t \in (0.01, 0.4)$. (a) Variation of exact expression $|a_2|$. (b) Error of $|a_2|$ in this paper.

their numerator and denominator defined in (13a) and (13b), respectively.

Using this result, we also calculated the absolute values of the coefficient $|a_2|$ and made a comparison on accuracies of the present results and the results published in [30], as shown in Fig. 5. It is seen in Fig. 5(a) that the coefficient $|a_2|$ is also monotonically changing and its magnitude is much smaller than that of $|a_1|$ by about ten times especially when the sphere core radius is electrically small or the nanoshell thickness is electrically very thin. Shown also in Fig. 5(b) is the relative error of the approximated a_2 values calculated using the approximate formulas in this paper. It is apparent that when the relative error of 0.15 is kept, the present formulas are quite accurate. Because the contribution of $|a_2|$ to the overall values of the extinction and scattering cross sections is only about 10%, so this makes the overall of the present error is even smaller.

B. Approximate Expression of Coefficient b_n

1) *Coefficient b_n* : Similarly, the coefficient b_n can be generally derived. However, it is realized that in many papers on nanoparticle scattering formulations, the coefficient b_n is not calculated at all. Nevertheless, the procedure for deriving the coefficients a_n and b_n in (4) is the same, also the formula structures for a_n and b_n are the same. Except for the change of the ratio m_3/m_2 in a_n into m_2/m_3 in b_n and the replacement of A_n in a_n by B_n in b_n symbolically, all the other formulations are identical. Therefore, we will not repeat this procedure, but simply provide the useful first-order coefficient b_1 for the comparison purpose.

By letting $n = 1$ in (4), we have the first term of the coefficient b_n simplified as

$$b_1 = y \frac{\beta_{1,n}}{\beta_{1,d}} \quad (25)$$

where

$$\begin{aligned} \beta_{1,n} = & -\frac{B_1 m_3^2}{m_2} + \frac{B_1 m_3^2}{6m_2} (m_3^2 - m_2^2) y^2 - \frac{B_1 m_3^2}{120m_2} \\ & \times (5m_2^4 - 6m_3^2 m_2^2 + m_3^4) y^4 + \frac{1}{45} m_2^2 m_3^2 (m_3^2 \\ & - m_2^2) y^5 + \frac{B_1 m_3^2}{15120m_2} (105m_2^6 + 63m_3^2 m_2^4 \end{aligned}$$

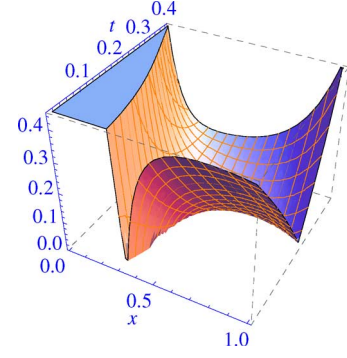


Fig. 6. Relative error (with respect to the exact solution) of the formulas $|b_1|$ derived in this paper versus the spherical core radius $x \in (0.01, 1.0)$ and the spherical nanoshell thickness $t \in (0.01, 0.4)$.

$$-9m_3^4 m_2^2 + m_3^6) y^6 \quad (26a)$$

$$\begin{aligned} \beta_{1,d} = & -\frac{iB_1 (m_2^2 - m_3^2)}{m_2 m_3} - \frac{im_2^3 + B_1 m_3^3}{m_2 m_3} y + \frac{iB_1}{2m_2 m_3} \\ & \times (m_2^4 - m_3^4) y^2 + \frac{i(m_2^2 - m_3^2)}{6m_2 m_3} (m_2^3 + iB_1 m_3^3) y^3 \\ & - \frac{iB_1}{48m_2 m_3} (m_2^2 - m_3^2)^3 y^4 + \frac{(m_2^2 - m_3^2)}{120m_2 m_3} (-im_2^5 \\ & + 5im_3^2 m_2^3 - 5B_1 m_3^3 m_2^2 + B_1 m_3^5) y^5 + \frac{1}{45} (m_2^2 m_3^4 \\ & - m_2^4 m_3^2) y^6. \quad (26b) \end{aligned}$$

In (25) together with (26a) and (26b), the parameter B_1 was defined in (14) ($n = 1$) together with their numerator and denominator defined in (17a) and (17b), respectively.

To check the accuracy, we have also calculated the coefficient b_1 . Shown in Fig. 6 is the relative error of b_1 values computed using the present solution in this paper. The parameters used in the calculations are the same as shown before in Figs. 4 and 5. It is seen clearly that when the relative error is controlled within 0.45, the area with high accuracy of the results in this paper is very large.

V. DISCUSSIONS AND CONCLUSION

The extinction total cross section (TCS) is defined as the ratio of the sum of absorbed and scattered energy of incident waves. Mathematically, the extinction TCS and the scattering cross section are expressed as

$$Q_{\text{ext}} = \frac{2\pi}{k_0^2} \sum_{n=1}^{\infty} (2n+1) \text{Re}[a_n + b_n] \quad (27a)$$

$$Q_{\text{sca}} = \frac{2\pi}{k_0^2} \sum_{n=1}^{\infty} (2n+1) [|a_n|^2 + |b_n|^2]. \quad (27b)$$

From these definitions, we could see that the closed-form expressions for the extinction cross section and the scattering cross section can be given analytically but approximately as follows:

$$Q_{\text{ext}} \approx \frac{2\pi}{k_0^2} [3\text{Re}[a_1] + 5\text{Re}[a_2] + 3\text{Re}[b_1]] \quad (28a)$$

$$Q_{\text{sca}} \approx \frac{2\pi}{k_0^2} [3|a_1|^2 + 5|a_2|^2 + 3|b_1|^2]. \quad (28b)$$

Apparently, these cross sections are dominated by the value of a_1 . The coefficients a_2 and b_1 also contribute to the extinction and scattering cross sections, and their contributions will improve the accuracy of calculating these cross sections although they are much smaller in value.

In summary, we have derived in this paper a new set of closed-form expressions of the classic Mie scattering coefficients of a spherical nanoshell using a power series up to order 6, which follows closely to the other set in [30]. The derived expressions are very general in nature, because the term number n of the Mie scattering coefficient series is still kept inside for the other potential applications, in addition to the general expressions consisting of the information of the three region electrical parameters (permittivities and permeabilities) and geometrical parameters (the electric inner and outer radii of the structure). This set of approximate expressions is found to be very accurate in the large range of various potential engineering applications including optical nanoparticle characterizations and other nanotechnology applications, validated step by step along the derivation procedure. Computations using this closed form of solutions are very fast and accurate for both lossy and lossless media, but it requires very little effort in the calculations of the cross-section results.

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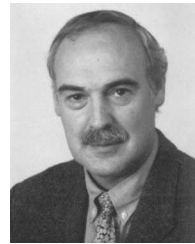


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